Launch of the ACE satellite

Intro. to Retrievals

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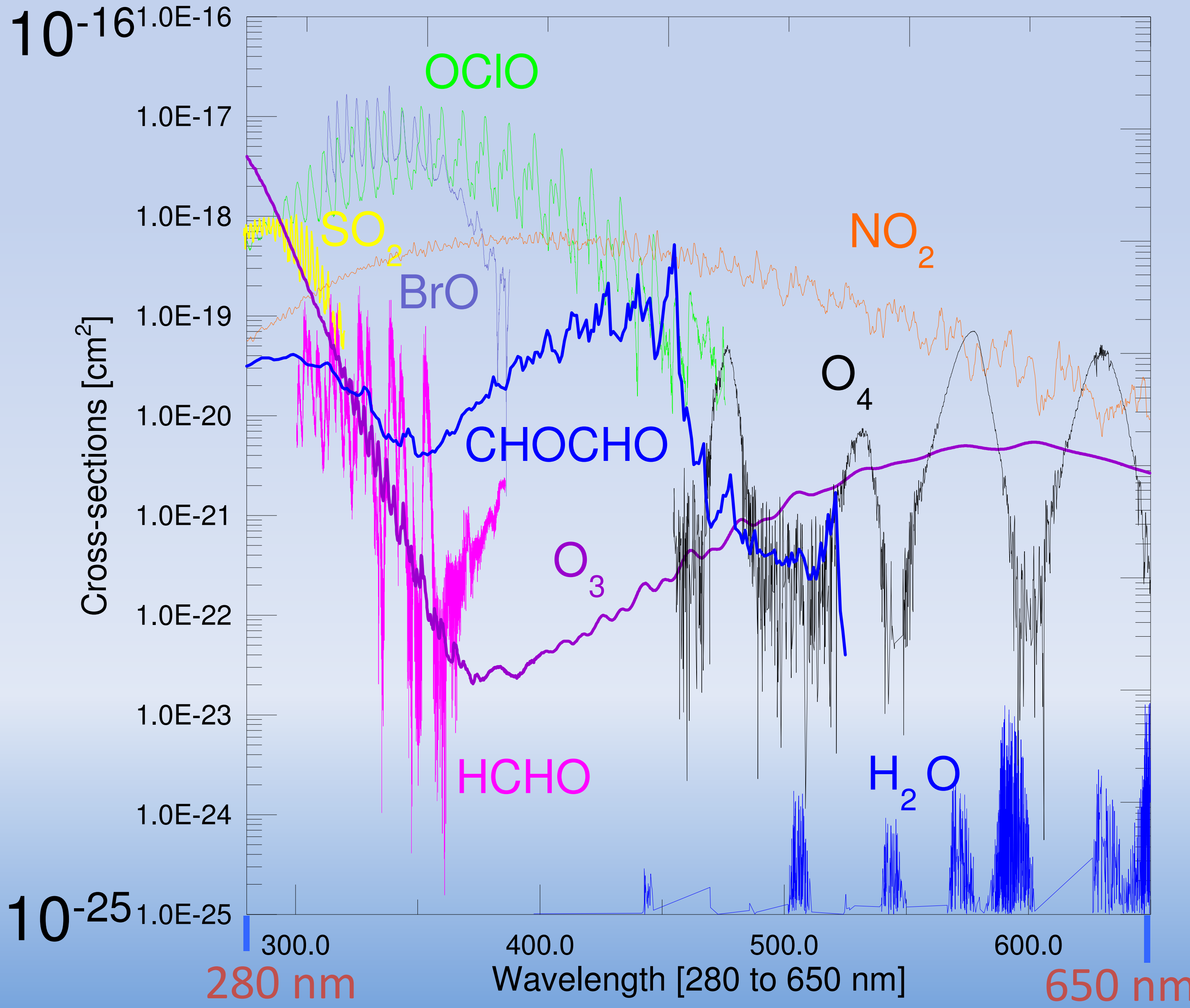
Topics for Today

- Cross-section spectra
- Example spectral detector
- A simple spectrometer
- Instrument characterization
- Spectral fitting
- Sample data
- More advanced techniques
- Conclusions

UVS Target Species

- O_3
- NO_2
- BrO
- OClO
- O_4
- H_2O
- HCHO
- CHOCHO
- Aerosol optical depth



“Two-component Instrument”

1. EG&G Reticon Detector

Detector: 1 inch long
1000 elements 0.001 inch each

0.1 inch

1 inch

Quantum efficiency peak 0.8 at ~750 nm
still useful ~0.3 down to 285 nm

Randomly Addressable

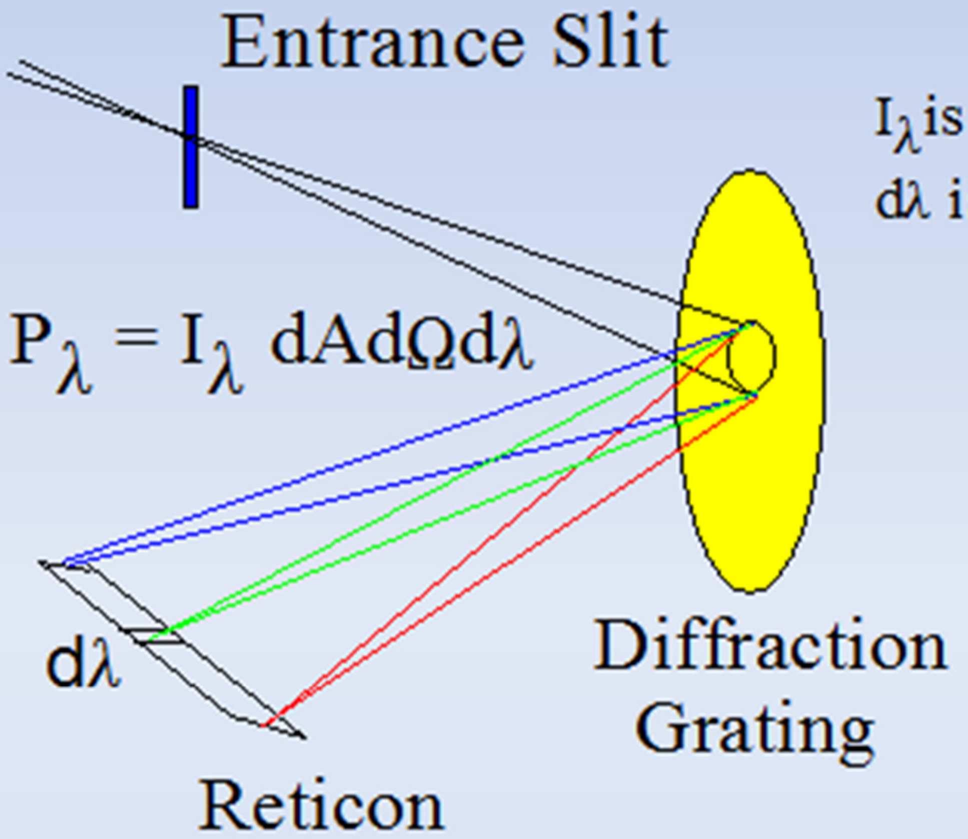
operate at short integration times
integration time to fit light intensity

2. Concave Holographic Grating

American Holographic

Grating First-Order Efficiency ~0.5

Diode-array Spectrometer



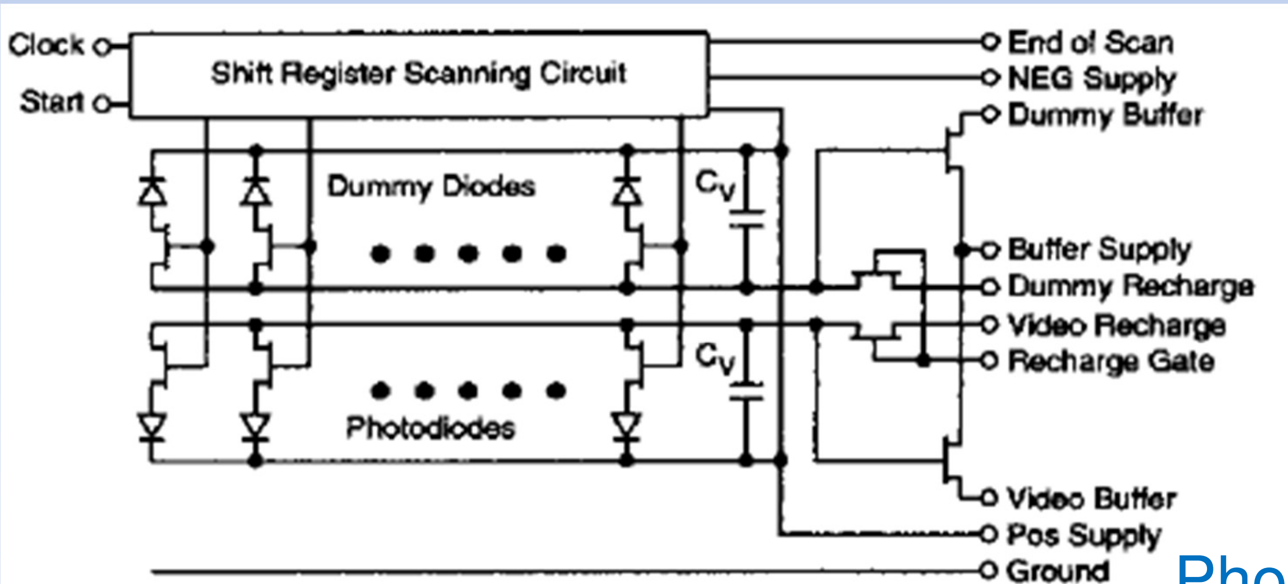
$P_\lambda = I_\lambda \, dA d\Omega d\lambda$

I_λ is solar intensity
$d\lambda$ is wavelength resolution

$dA = l \cdot w$
where l = slit length
and w = slit width

$d\lambda = D \cdot w$
where D is the dispersion
and w is the slit width

RETICON Detector



Pixels are charged to a reference level & isolated by transmission gates

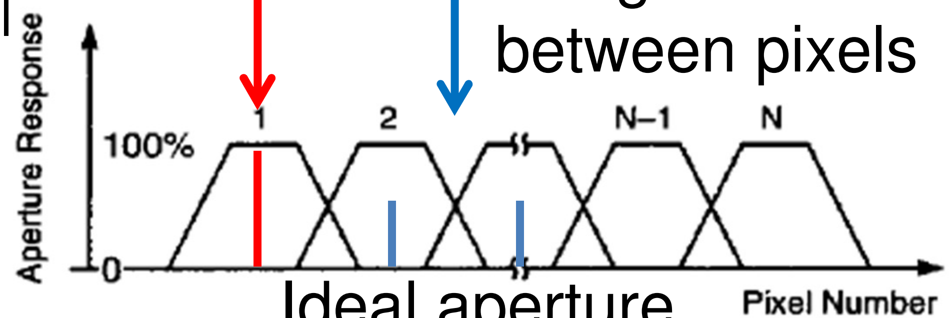
Light causes the capacitance of the photodiodes to discharge

The number of electrons to recharge the pixel is measured

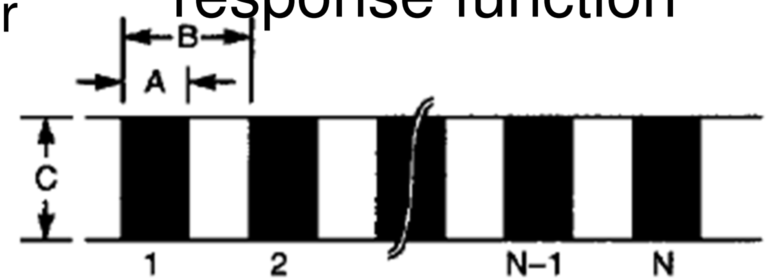
The result digitized and stored by computer

Photons

Charge is shared between pixels

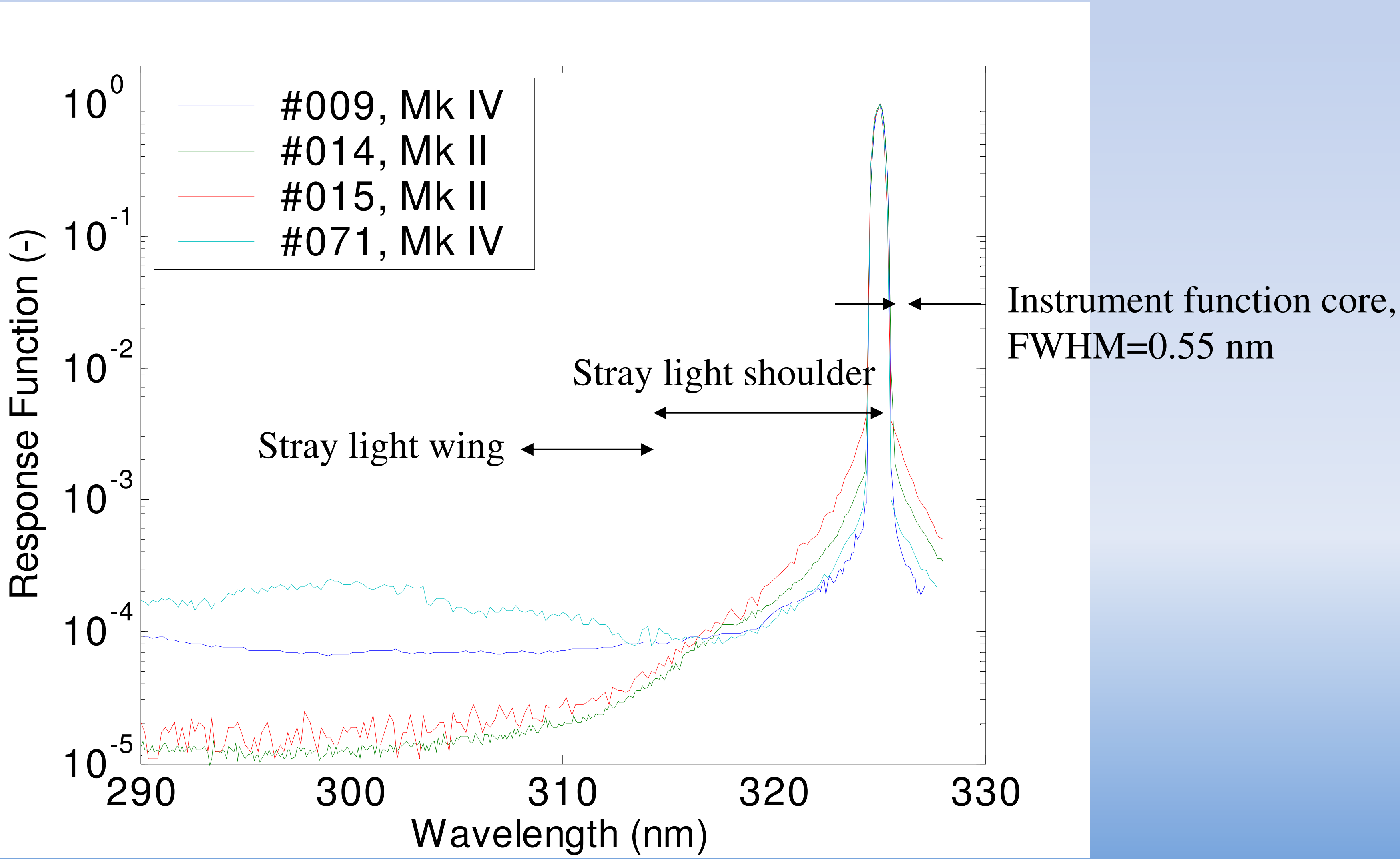


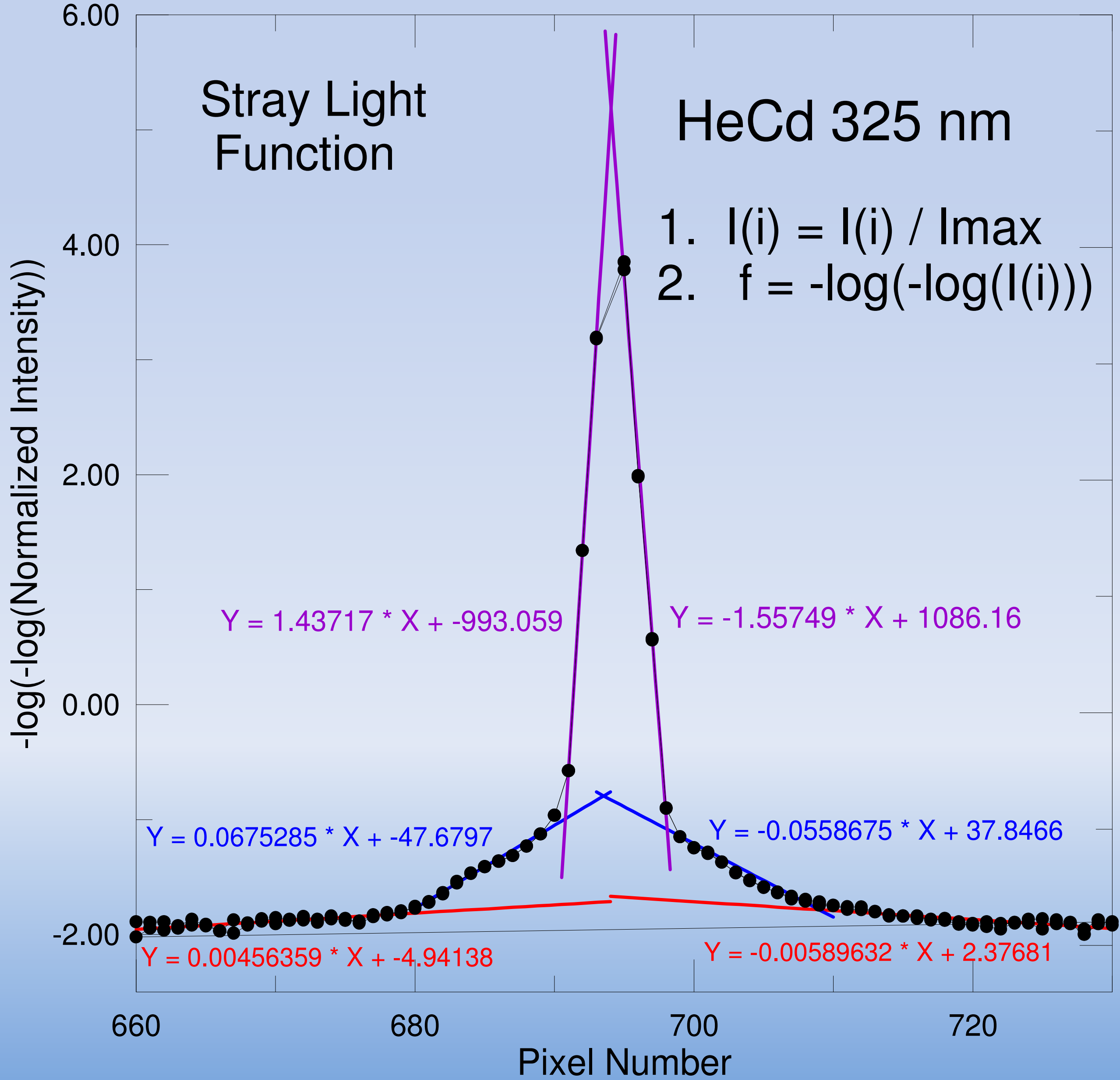
Ideal aperture response function



Laserscans

Single-Brewer stray light rejection is 10^{-5}-10^{-4} as measured by scanning 325 nm HeCd laserline





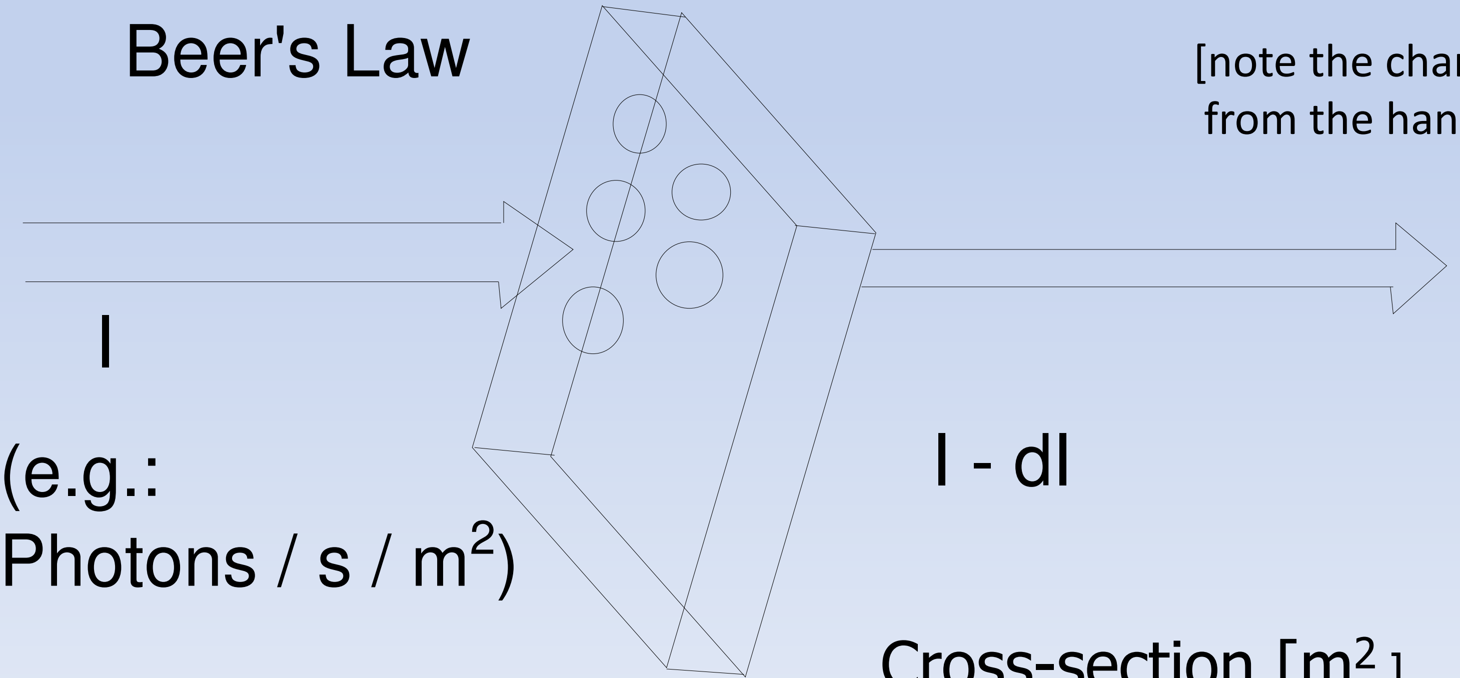
CPFM Stray Light Function

Composition and Photodissociative Flux Measurement

Beer's Law

Beer's Law

[note the changes from the handout]



I

(e.g.: Photons / s / m^2)

$I - dI$

Cross-section [m^2]

$dI(\lambda) = I(\lambda)\,\sigma(\lambda)\,\rho\,ds == I(\lambda)\,d\tau$

σ – cross-section [m^2]

$dI/I = -\,d\tau$ Integrated: $I = I_o e^{-\tau}$

ρ – number density [m^{-3}]

ds – differential length [m]

Or $\tau = \log[\ I_o(\lambda)\ ] - \log[\ I(\lambda)\ ]$

Where I_o is incident intensity

T – optical depth

Notation

$$\sum_{j=0}^{j<N_c} x_j \, y_j$$

Sum of $x_0 \, y_0 + x_1 \, y_1 + \ldots + x_{N-1} \, y_{N-1}$
Also $x_j \, y_j$ with repeated subscript convention
(sometimes called the Einstein convention)

Covariance

$$\sigma_{jk} = \sum \, (x_{ij} - \overline{x}_j) \, (x_{ik} - \overline{x}_k)$$

With mean:

$$\overline{x}_j = \frac{1.0}{N_i} \sum_{i=0}^{i<N_i} x_{ij}$$

But frequently x_i and x_j are considered uncorrelated and σ diagonal

Spectral Fitting

$I(\lambda_i) = \int I(\lambda)\, S(\lambda - \lambda_i)\, d\lambda$

$C(\lambda_i) = R_i\, I(\lambda_i)$

$I(\lambda) = I_o(\lambda) \exp[\, -\tau(\lambda)\,]$

$\tau(\lambda) = \tau_c(\lambda) + \tau_R(\lambda) + \tau_a(\lambda)$

Clearly, since:

$I(\lambda)$ – light intensity

λ_i effective wavelength of pixel i

$S(\lambda)$ – slit function

R_i – response of pixel i

$I_o(\lambda)$ – source intensity

$\tau(\lambda)$ – optical depth

c – constituents

R – Rayleigh (air)

a – aerosol (particles)

$$\exp[\, -\tau(\lambda)\,] = \exp[\, -\tau_c(\lambda)\,]\, \exp[\, -\tau_R(\lambda)\,]\, \exp[\, -\tau_a(\lambda)\,]$$
$$= \exp\{\, -[\tau_c(\lambda) + \tau(\lambda)_R + \tau(\lambda)_a]\, \}$$

Absorbers

$$\tau_c(\lambda) = \sum_{j=0}^{j<N_c} \sigma_j(\lambda)\, \eta_j$$

$\sigma_j(\lambda)$ – cross-section molecule j

η_j – column density [molec/cm^2]

N_c – number of absorbers

$\rho_j(s)$ – density of constituent j

$$\eta_j = \int_s \rho_j(s)\, ds$$

$$I(\lambda_i) = \int I_o(\lambda) \exp[-\sigma_j(\lambda)\, \eta_j]\, S(\lambda - \lambda_i)\, d\lambda \quad \text{sum over j}$$

One approach to fitting the spectrum is to minimize
The log-difference between the model and the
measurements (m):

$$SE = \sum_{i=0}^{i<N_\lambda} \{ \log[I^m(\lambda_i)] - \log[I(\lambda_i)] \}^2$$

Solution

Let $L(\lambda_i) == \log[\, I(\lambda_i)\,]$ Then the square difference becomes:

$$SE = \sum_{i=0}^{i < N_\lambda} [\, L^m(\lambda_i) - L(\lambda_i)\,]^2$$

SE depends on the amount of the various absorbers. An estimate of the amounts can be done by minimizing SE with respect to the different constituents.

$$\frac{\partial SE}{\partial \eta_c} = \sum_{i=0}^{i < N_\lambda} 2\, \frac{\partial L(\lambda_i)}{\partial \eta_c}\, [\, L^m(\lambda_i) - L(\lambda_i)\,] == 0.0$$

At some point there will be a set of η_c producing a log spectrum $L(\lambda_i)$ which is not the best fit to $L^m(\lambda_i)$

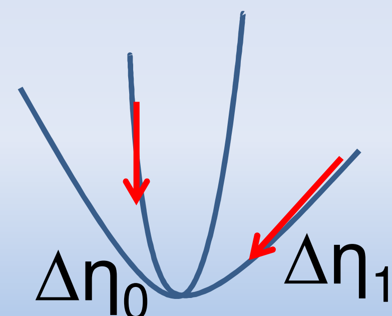
Equation

Assume $\Delta L(\lambda_i) = [\ L^m(\lambda_i) - L(\lambda_i)\ ]$

$$\frac{\partial SE}{\partial \eta_c} = \sum_{i=0}^{i<N_\lambda} \frac{\partial L(\lambda_i)}{\partial \eta_c} \Delta L(\lambda_i) \text{ near } 0.0$$

Make a small displacement in η_c ($\Delta\eta_c$) to make the sum smaller:

$$\delta L(\lambda_i) = \frac{\partial L(\lambda_i)}{\partial \eta_k} \Delta\eta_k$$



$$\sum_{i=0}^{i<N_\lambda} \frac{\partial L(\lambda_i)}{\partial \eta_c} \left[\Delta L(\lambda_i) - \frac{\partial L(\lambda_i)}{\partial \eta_k} \Delta\eta_k \right] == 0.0$$

Matrix

$$\sum_{i=0}^{i<N_\lambda} \frac{\partial L(\lambda_i)}{\partial \eta_c} \frac{\partial L(\lambda_i)}{\partial \eta_k} \Delta\eta_k = \sum_{i=0}^{i<N_\lambda} \frac{\partial L(\lambda_i)}{\partial \eta_c} \Delta L(\lambda_i)$$

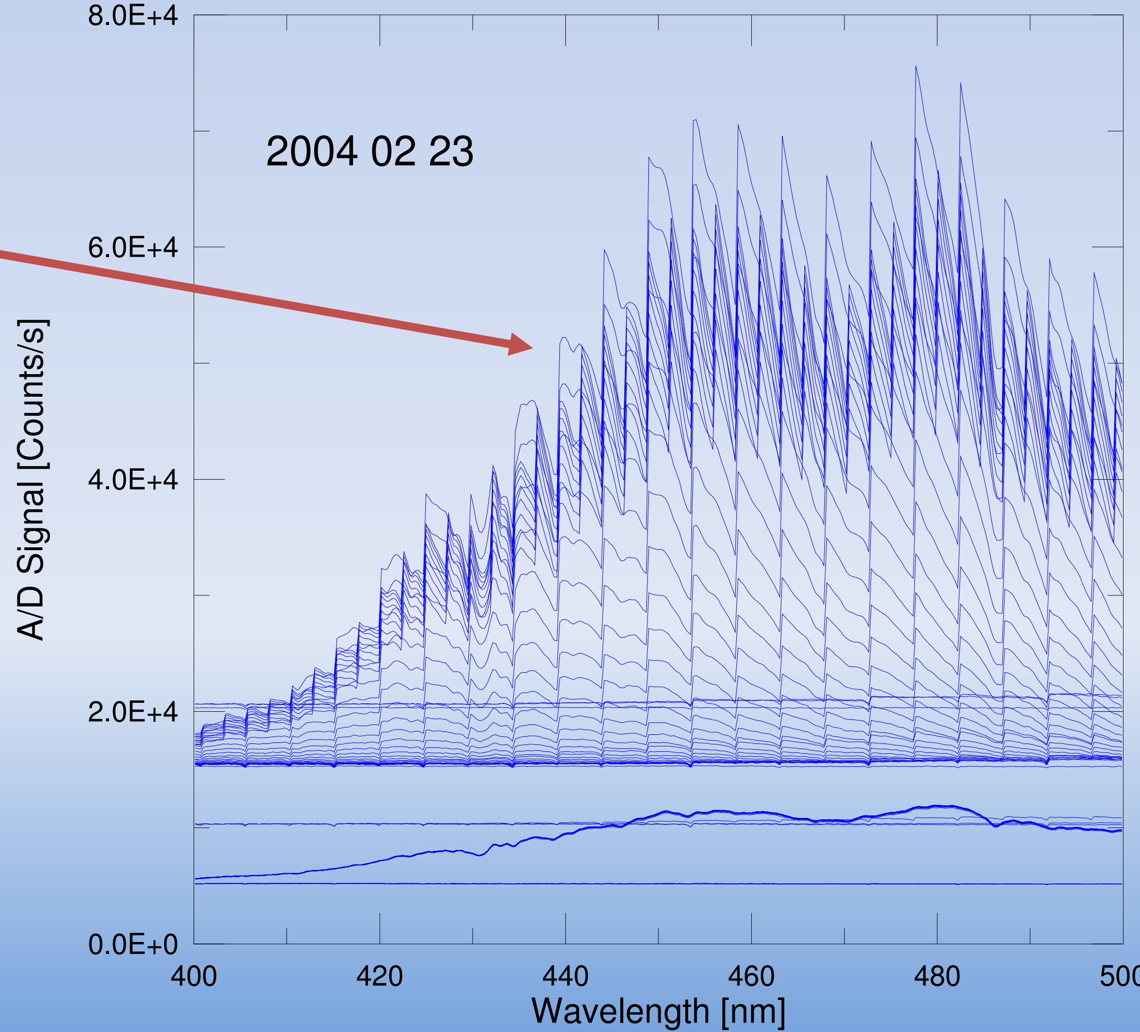
Let $$K_{ck} = \sum_{i=0}^{i<N_\lambda} \frac{\partial L(\lambda_i)}{\partial \eta_c} \frac{\partial L(\lambda_i)}{\partial \eta_k}$$

and $$Y_c = \sum_{i=0}^{i<N_\lambda} \frac{\partial L(\lambda_i)}{\partial \eta_c} \Delta L(\lambda_i)$$

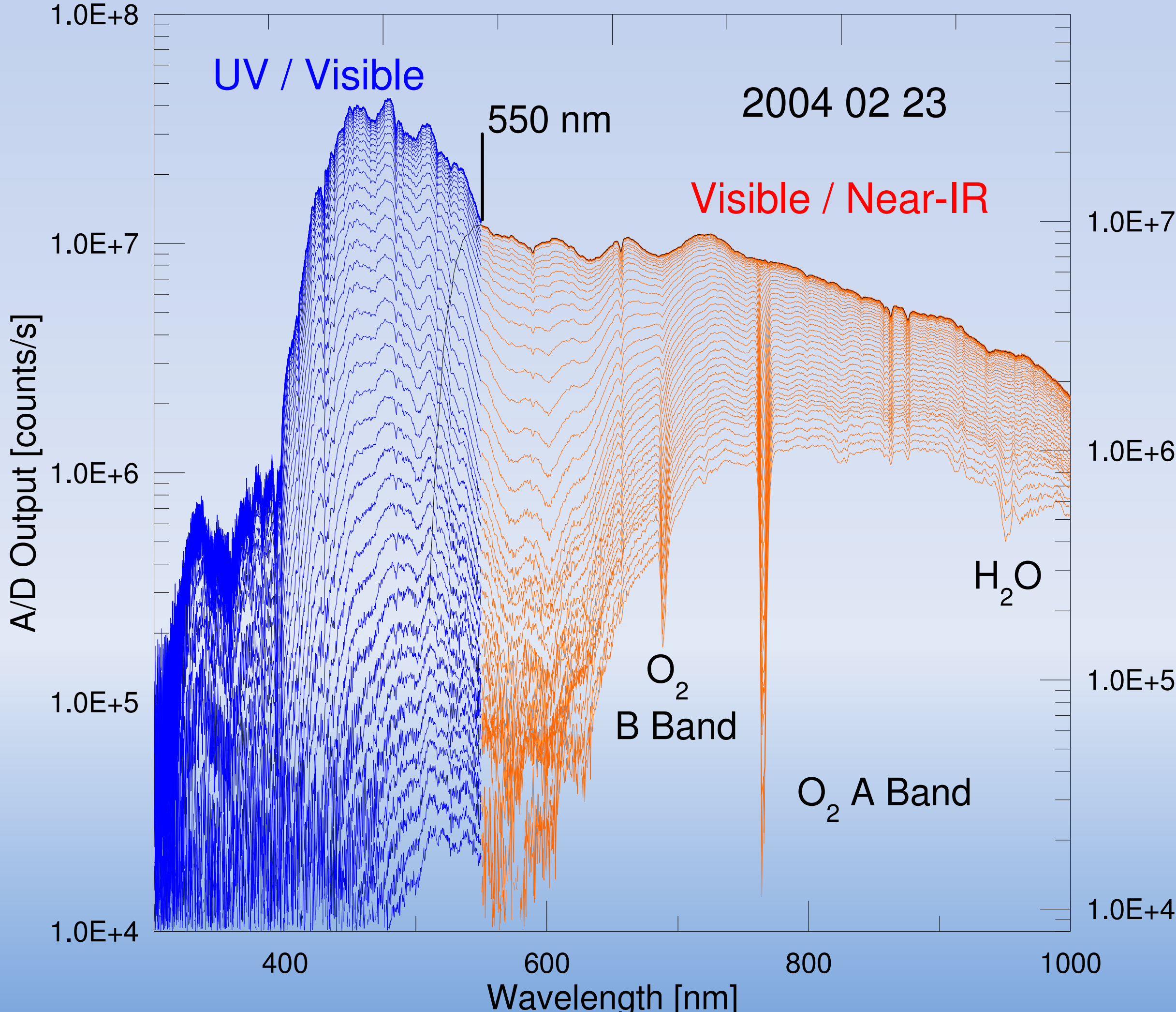
$$K_{ck} \Delta\eta_k = Y_c \qquad \Delta\boldsymbol{\eta} = \mathbf{K}^{-1}\,\mathbf{Y}$$

Raw Data
Vis Spectrometer

The observing strategy attempts to keep the detector wells full…



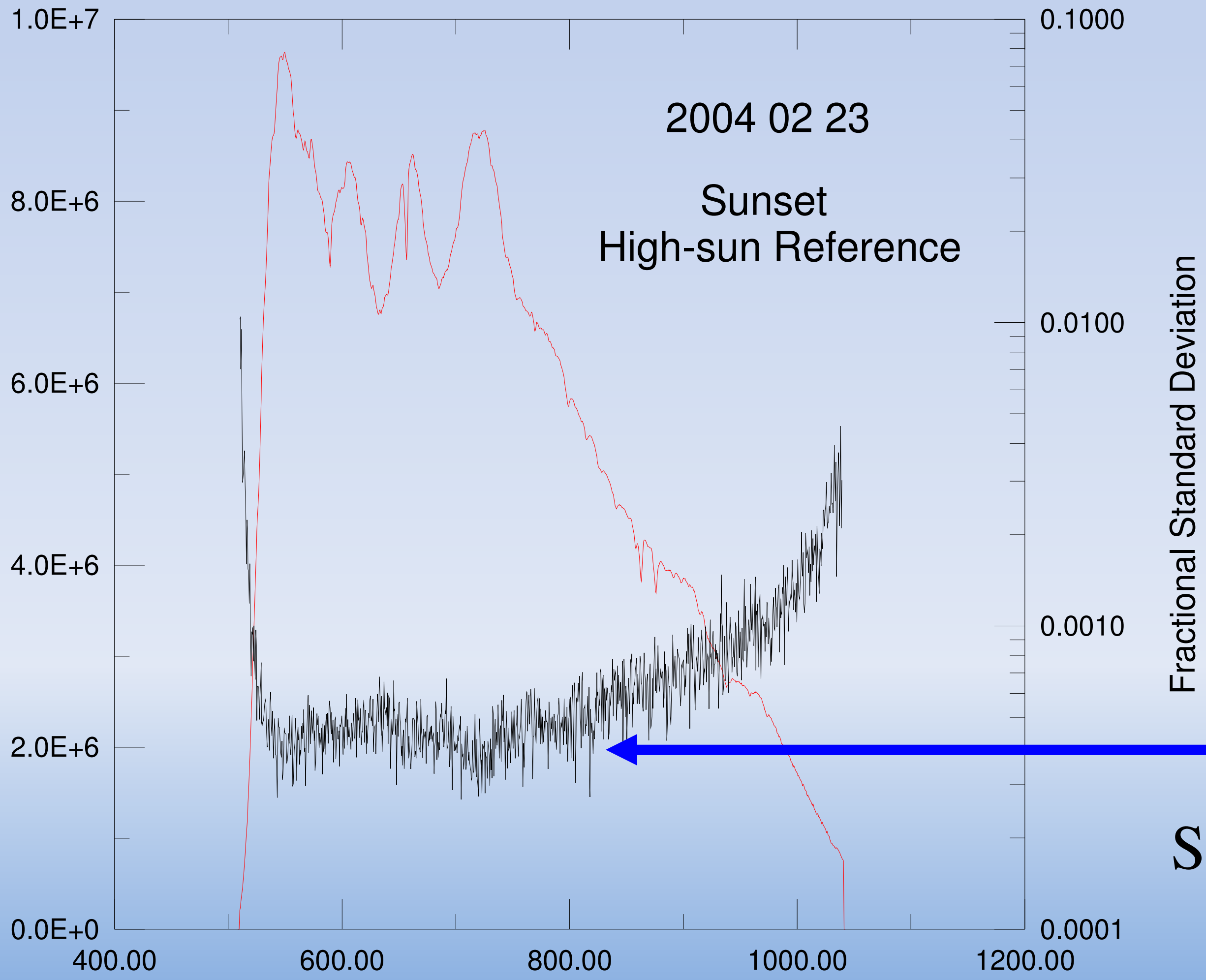
Real Data - Counts/s



After dark count and stray light correction, scale to counts per second…

Note: Axes are shifted to line up the brightest spectra in the UV and Visible. All others line up because of the high linearity of the systems.

ETS & Fractional Uncertainty

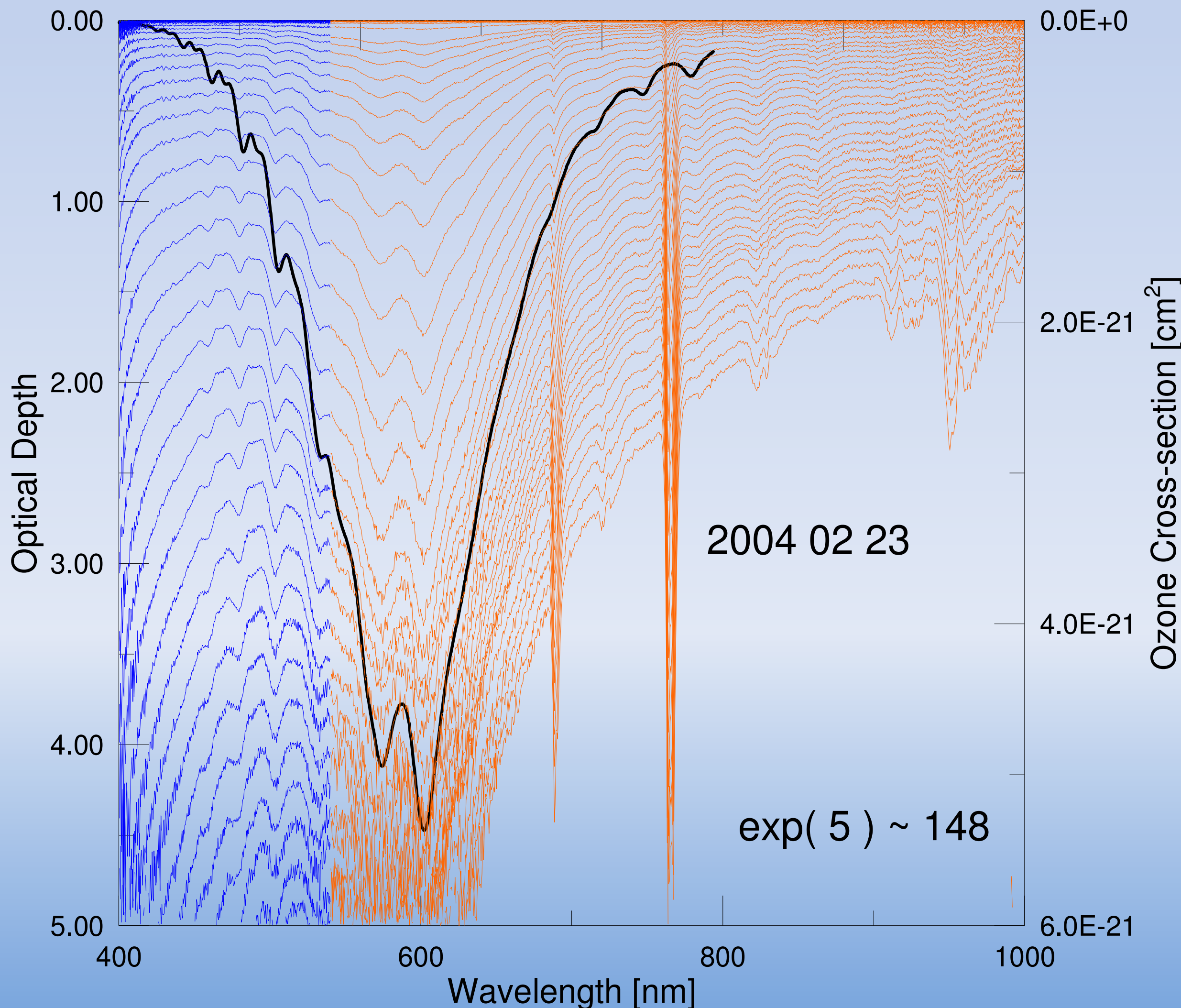


Mean ETS from ~21 spectra

$4x10^{-4}$ RMS

STD ERROR $9x10^{-5}$

Optical Depth



A mean reference spectrum from 15 high-sun spectra is used to estimate wavelength-dependent optical depth

These apparent optical depth spectra are fitted to determine constituent surface densities (slant columns)

n^{th} Iteration, Analytic Derivative

$$\eta_k^{n+1} = \eta_k^n + \Delta\eta_k$$

Remember? (This is where the magic happens)

$$I(\lambda_i) = \int I_o(\lambda) \exp[\, -\sigma_j(\lambda)\, \eta_j\,]\, S(\lambda - \lambda_i)\, d\lambda \quad \text{sum over } j$$

$$L(\lambda_i) = \log[\, I(\lambda_i)\,]$$

Definition of log(): $d\log(x) = dx/x$

$$\frac{\partial L(\lambda_i)}{\partial \eta_k} = \frac{1.0}{I(\lambda_i)} \frac{\partial}{\partial \eta_k} \int I_o(\lambda) \exp[\, -\sigma_j(\lambda)\, \eta_j\,]\, S(\lambda - \lambda_i)\, d\lambda$$

Analytic Derivatives

Discrete v. Analytic Derivatives

Discrete: $\frac{\partial y}{\partial x} = [\ y(\ x + \Delta x) - y(\ x\ )\ ] / \Delta x$

The problem: if Δx is too big the slope isn't appropriate to y(x)

If Δx is too small the differential is all noise.

The analytic approach avoids this.
It also calculates everything in one pass of the forward model instead of N + 1 passes.

Result…

$$\frac{\partial L(\lambda_i)}{\partial \eta_k} = \frac{1.0}{I(\lambda_i)} \frac{\partial}{\partial \eta_k} \int I_o(\lambda)\ \exp[\ -\sigma_j(\lambda)\ \eta_j\ ]\ S(\lambda - \lambda_i)\ d\lambda$$

$$= \frac{1.0}{I(\lambda_i)} \int\ I_o(\lambda) \frac{\partial}{\partial \eta_k} \{\ \exp[\ -\sigma_j(\lambda)\ \eta_j\ ]\ \}\ S(\lambda - \lambda_i)\ d\lambda$$

$$= -\frac{1.0}{I(\lambda_i)} \int I_o(\lambda)\ \sigma_k(\lambda)\ \exp[\ -\sigma_j(\lambda)\ \eta_j\ ]\ S(\lambda - \lambda_i)\ d\lambda$$

Remember?

$$L(\lambda_i) = \log\{ \int I_o(\lambda)\ \exp[\ -\sigma_j(\lambda)\ \eta_j\ ]\ S(\lambda - \lambda_i)\ d\lambda\ \}$$

So many of the terms in the differentials are already being calculated for the intensity spectrum.

Numerology

We don't actually measure an infinite number of wavelengths
So the integral form doesn't really apply:

$$I(\lambda_i) = \int I_o(\lambda)\ \exp[\ -\sigma_j(\lambda)\ \eta_j\ ]\ S(\lambda - \lambda_i)\ d\lambda \quad \text{sum over j}$$

So the equation becomes

$$I(\lambda_i) = \sum_{l=0}^{l<N_\lambda} I_o(\lambda_l)\ \exp[\ -\sigma_j(\lambda_l)\ \eta_j\ ]\ S(\lambda_l - \lambda_i) \qquad \text{sum over j}$$

And a similar expression for the differential:

$$\frac{\partial I(\lambda_i)}{\partial \eta_k} = \sum_{l=0}^{l<N_\lambda} I_o(\lambda_l)\ \sigma_k(\lambda_l)\ \exp[\ -\sigma_j(\lambda_l)\ \eta_j\ ]\ S(\lambda_l - \lambda_i)$$

Where the spacing of λ_l is small enough for an accurate result

Practical

- The preceding development did not consider noise
- But different parts of the spectrum have different noise
- It is also desirable to estimate the uncertainty in the result
- Rather than minimizing the square error, one can use X^2

$$\text{Let} \qquad \Delta_i = \log[\, I^m(\lambda_i)\,] - \log[\, I(\lambda_i)\,]$$

$$X^2 = \sum_{i=0} \sum_{j=0} \Delta_i \, \sigma_{ij}^{-1} \Delta_j$$

σ is the error covariance matrix
and is frequently taken to be diagonal i.e.: in this case the individual wavelength's noise is considered to be uncorrelated

Comments

Easy to show that if the noise on the observations is well represented by σ, then each degree of freedom (e.g. each x_j) should multiply to 1.0 so that X^2 will have a value equal to the number of degrees of freedom.

Scaling by σ^{-1} normalizes the scatter of each of the dimensions of the x_{ij}. The departure of the value of X^2 from the number of degrees of freedom is a measure of how well the model fits the data.

More Advanced Methods

It is possible to generate X^2 terms that constraint solutions in other ways for example:

- Prior knowledge of mean and covariance
- Smoothing terms with uncertainty matrix
- Functional constraints

This is the basis of the Rodgers optimal estimation technique

The individual terms are all of order unity per degree of freedom and can be summed and simultaneously minimized

Wavelength shift and stretch can also be simultaneously retrieved

Other Independent Variables

Wavelength shift and Stretch:

$$\lambda' = \lambda + \text{shift} + \text{stretch} * (\lambda - \lambda_c)$$

$$\partial I/\partial \text{shift} = \partial I/\partial \lambda$$

$$\partial I/\partial \text{stretch} = \partial I/\partial \lambda \, (\lambda - \lambda_c)$$

$\partial I/\partial \lambda$ can be determined by differentiating the interpolation routine used to interpolate $I(\lambda)$

Cross-section temperature effects:

$$\sigma(\lambda , T) = \sigma(\lambda, T_o) + \partial \sigma/\partial T \, (T - T_o)$$

$$I = I_o \exp(- \sigma(\lambda , T) X); \quad \log(I) = \log(I_o) - \sigma(\lambda , T) X$$

$$\log(I) = \log(I_o) - \underline{\sigma(\lambda , T_o)} \, \underline{X} - \underline{\partial \sigma/\partial T} \, \underline{(T - T_o) X}$$

Conclusion

Any instrument will respond to a number of inputs

e.g. light from the wrong wavelengths
thermal and pressure effects
thermally generated photons
non-linearity
mechanical vibration or stress
signal ‘memory’
sensitivity drift
radiation effects

The experimentalist’s job is to isolate the effects, model them properly and use as few retrievable parameters as possible to account for them. Ideally the ‘raw’ data should be fitted with a model.

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nrise during the
Arctic Campaign
unrise 2010
The End. Thank you.

Lessons One

1. Thou shalt NOT build computers. IBM can lose money at it, and you can use up ALL your resources accomplishing the goal of delivering late, a computer which was built from obsolete components. The OEM's corner the market on the up-to-date stuff.

2. Don't run anything on batteries. If there is an outlet -- plug in to it. If there is no outlet, have one installed.

3. Every instrument needs a parent. Don't let one drift along as an orphan -- it will wind up as a juvenile delinquent and embarrass you later on.

4. If a project appears to be difficult, either cancel it or provide the resources needed for it. Half-assed management leads to a half-assed project.

5. Almost ANY amount of paperwork is easy compared to making more hardware [see 1]. (i.e.: if a computer already exists -- use it.)

6. Never make a half-dozen, make a dozen. Especially if you can avoid making bits you don't have to make.

Lessons 1 con't

7. Don't use matrix management without accountability. People see things as important if they are personally involved -- one way or another.

9. Above all - don't say yes to running a project over which you have no control!

10. If you are responsible for a project someone else is managing, try to remove obstacles from the path -- don't add sand traps and rough ground.

11. If you change managers, especially if you do so because of perceived problems in the development process, do the whole design over again. Salvage what you can, but be sure that there were no endemic problems which lead to the superficial symptoms.

12. Use benchmarks along the way to develop schedules, and then meet some of the deadlines along the way. Otherwise nothing gets done. Don't manage part of the project, or part of the time of the involved principals, because the other demands on the people will make it impossible to meet deadlines.

Lessons Two

Don’t do space experiments; but if you do…

Be somewhat conservative in technology steps

To quote Jim Drummond: Test as you fly (the whole thing!)
Recognize the difference between:

- Functionality tests
- Tests showing contractual compliance
- Tests showing science output
- Characterization

If an unplanned procedure has to be implemented have all the stakeholders on site for the operation. Different folks see different things.

Engineering is the art of never again making a mistake you have already made before. Space experiments are harder.